Photoinduced Dynamics of the Finite Size 2D Hubbard Model

P04

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TU Graz

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TU Graz

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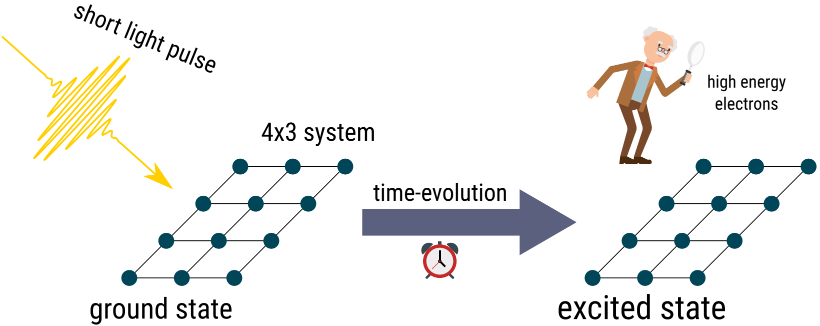
Simulation Goal



Model

Hubbard model

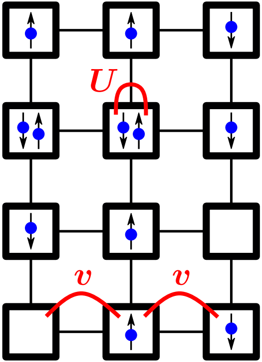
$$H = H_{hop} + H_{loc}$$

Kinetic energy, hopping

$$H_{hop} = -\sum_{\langle ij\rangle,\sigma} v_{ij}\; c^{\dagger}_{i,\sigma} c_{j,\sigma} \;+\; v^{*}_{ij}\; c^{\dagger}_{j,\sigma} c_{i,\sigma}$$

Potential energy, Coulomb interaction

$$H_{loc} = U \sum_{i} \left(n_{i,\uparrow} - \frac{1}{2}\right)\left(n_{i,\downarrow} - \frac{1}{2}\right)$$



How to Simulate Photons? $\longrightarrow$ Peierls Approximation

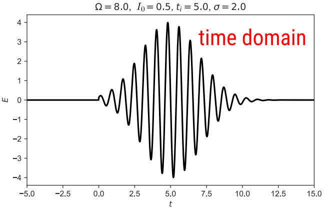
$$H_{hop} = -\sum_{\langle ij\rangle,\sigma} v_{ij}\ c^\dagger_{i,\sigma} c_{i,\sigma} + v^*_{ij}\ c^\dagger_{j,\sigma} c_{j,\sigma}$$

$$v_{ij} \longrightarrow v_{ij}\ e^{\mathrm{i} \int_{\boldsymbol{x}_i}^{\boldsymbol{x}_j} \boldsymbol{A}(\boldsymbol{x},t)\ \mathrm{d}\boldsymbol{x}} \qquad \text{(Peierls phase)}$$

We choose the electric field $\boldsymbol{E} = -\frac{\partial \boldsymbol{A}}{\partial t}$, so that

$$\int_{\boldsymbol{x}_i}^{\boldsymbol{x}_j} \boldsymbol{A}(\boldsymbol{x},t)\ \mathrm{d}\boldsymbol{x} = -I_0\ e^{-\frac{(t-t_i)^2}{2\sigma^2}}\ \left(\cos\left(\Omega\left(t-t_i\right)\right) - \cos\left(-\Omega\ t_i\right)\right)$$

$$\sigma = 2.0 \qquad t_i = 5.0$$



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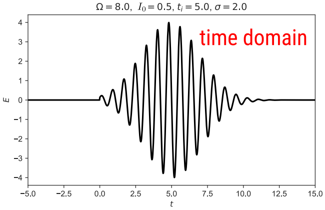

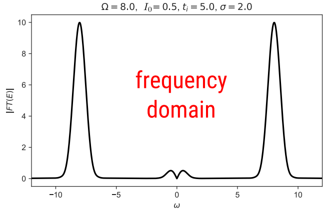

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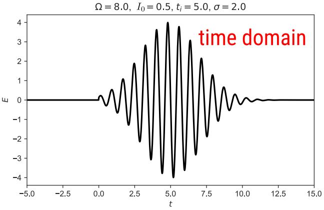
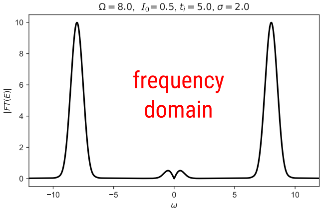
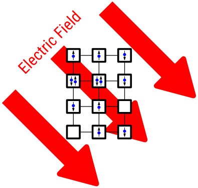
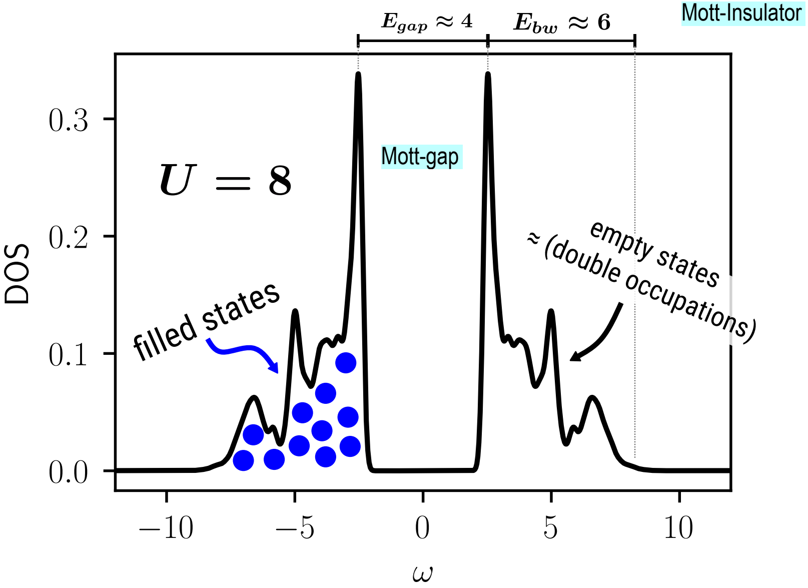


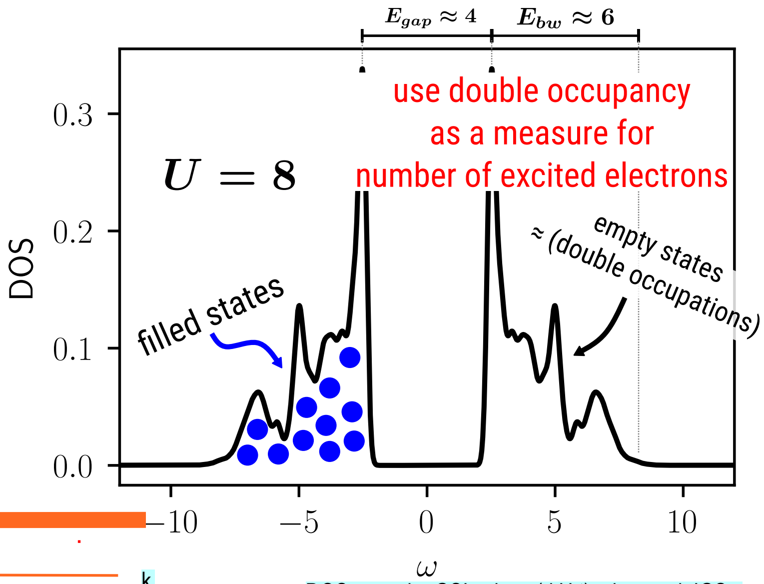




Density of States (4×3 Hubbard Model)



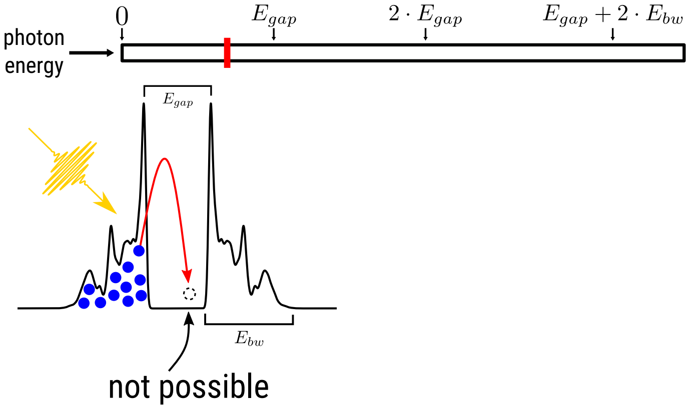
Density of States (4 × 3 Hubbard Model)



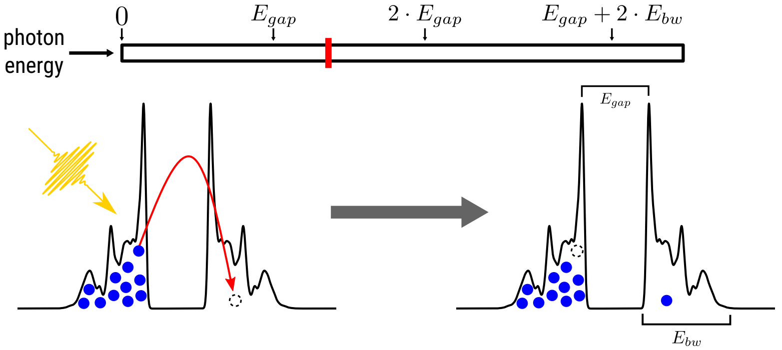
k

DOS: sum_j <GSI c_j exp(-i H t) cdagger_j IGS>

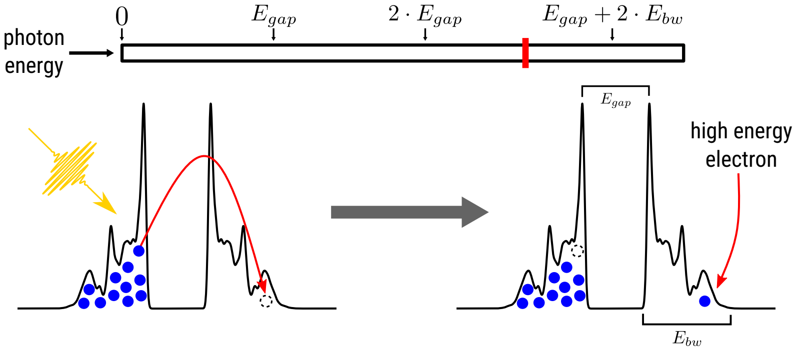
Photon Absorption: Very Low Energy



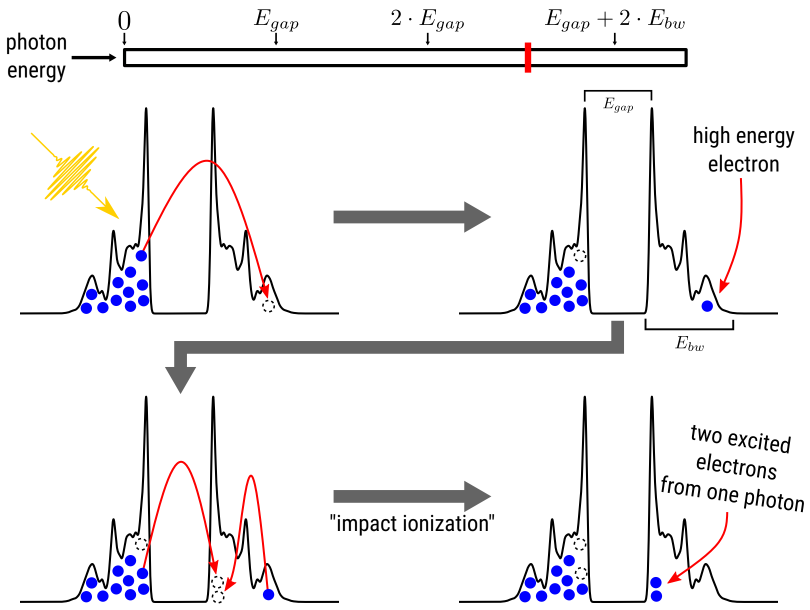
Photon Absorption: Low Energy



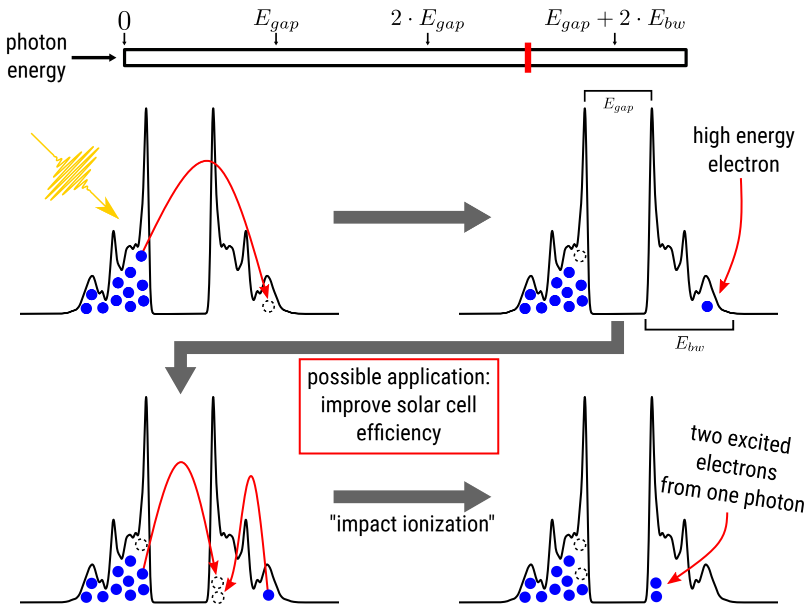
Photon Absorption: High Energy



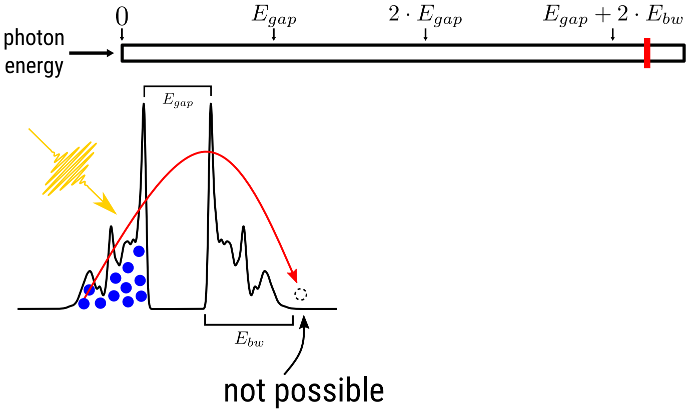
Photon Absorption: High Energy



Photon Absorption: High Energy



Photon Absorption: Very High Energy



Method

4×3 Hubbard model $\longrightarrow$ 853776 eigenstates (too many for ED).

Half filling: 6 up spins on 12 sites and 6 down spins on 12 sites

Simulation:

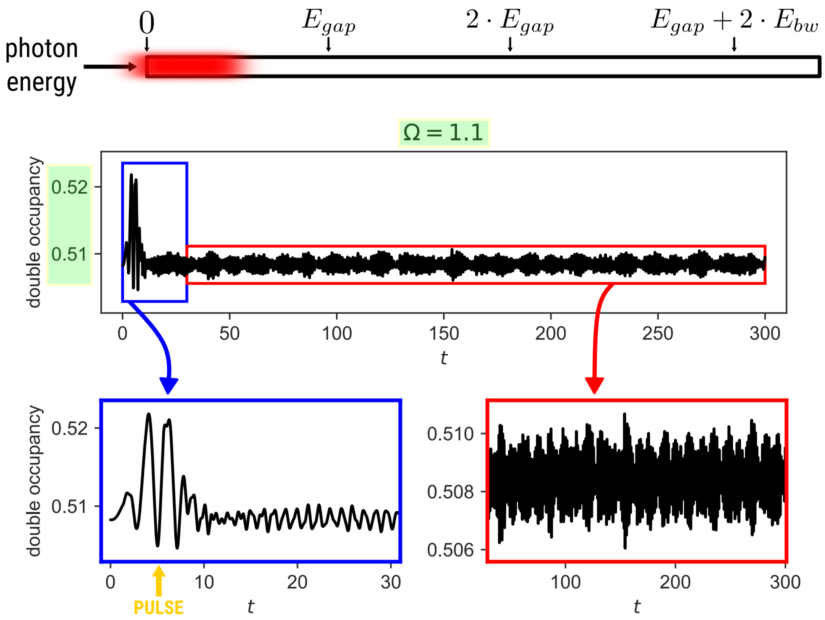
- Initial state: ground state $|\psi(0)\rangle$ computed with Lanczos method. similar Conjugate Grad.

- $|\psi(t+\Delta t)\rangle = e^{-\mathrm{i}\,H(t)\,\Delta t}\,|\psi(t)\rangle$ approx (1 - i H Delta_t) / psi(t) >
  is computed in Krylov subspace of $|\psi(t)\rangle$.

  Krylov subspace of $|\psi(t)\rangle$: $\mathrm{span}\{|\psi(0)\rangle\,, H\,|\psi(0)\rangle\,, H^2\,|\psi(0)\rangle\,, \ldots\}$

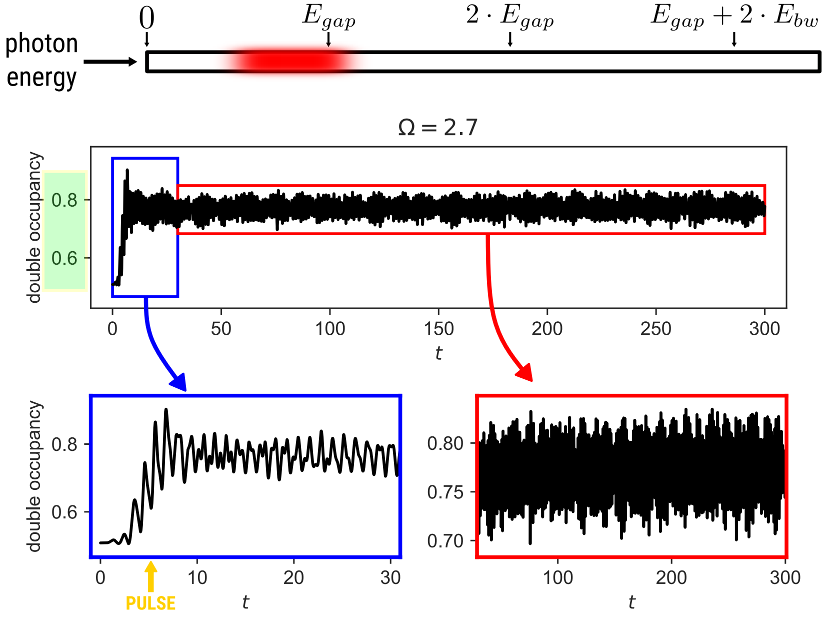
- very accurate

Results



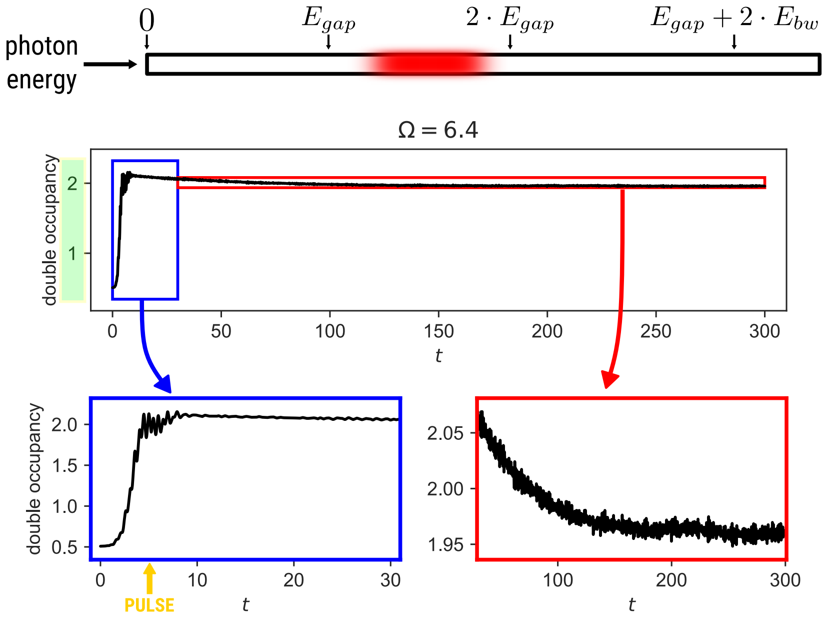
0
E_{gap}
$2 \cdot E_{gap}$
$E_{gap} + 2 \cdot E_{bw}$
photon energy
$\Omega = 1.1$
double occupancy
0.52
0.51
0
50
100
150
200
250
300
t
double occupancy
0.52
0.51
0
10
20
30
PULSE
t
0.510
0.508
0.506
100
200
300
t

Results



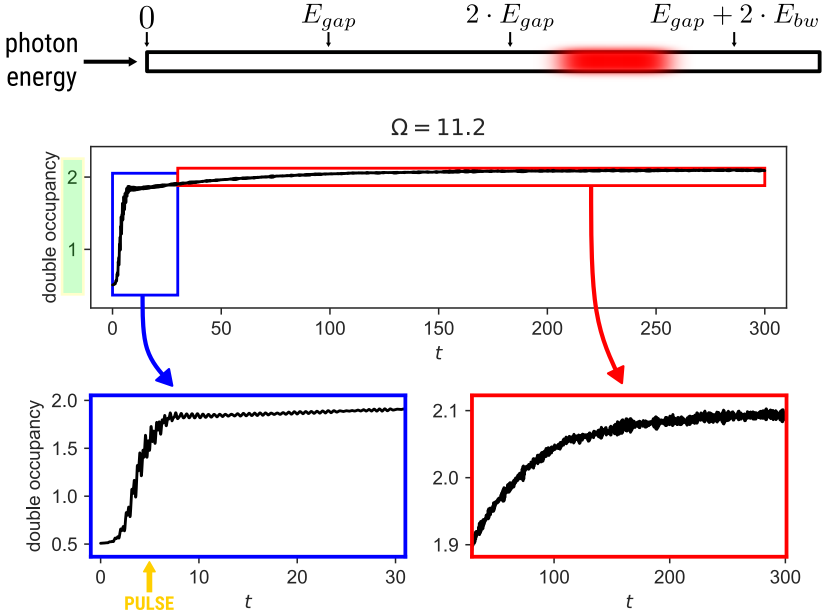
0
E_{gap}
$2 \cdot E_{gap}$
$E_{gap} + 2 \cdot E_{bw}$
photon
energy
$\Omega = 2.7$
double occupancy
0.8
0.6
0
50
100
150
200
250
300
t
double occupancy
0.8
0.6
0
10
20
30
PULSE
t
0.80
0.75
0.70
100
200
300
t

Results



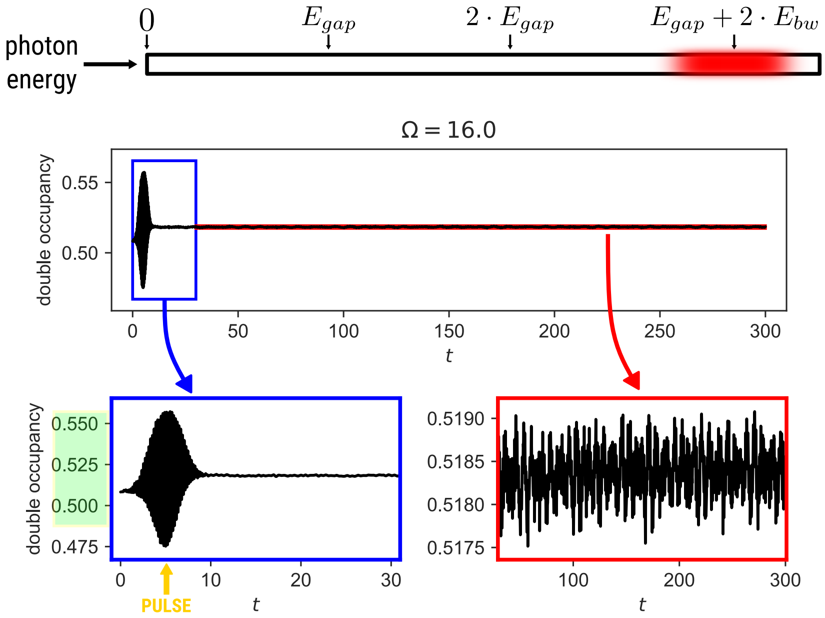
0
E_{gap}
$2 \cdot E_{gap}$
$E_{gap} + 2 \cdot E_{bw}$
photon energy
$\Omega = 6.4$
double occupancy
2
1
0
50
100
150
200
250
300
t
double occupancy
2.0
1.5
1.0
0.5
0
10
20
30
PULSE
t
2.05
2.00
1.95
100
200
300
t

Results



photon energy
0
E_{gap}
$2 \cdot E_{gap}$
$E_{gap} + 2 \cdot E_{bw}$
$\Omega = 11.2$
double occupancy
2
1
0
50
100
150
200
250
300
t
2.0
1.5
1.0
0.5
10
20
30
PULSE
2.1
1.9

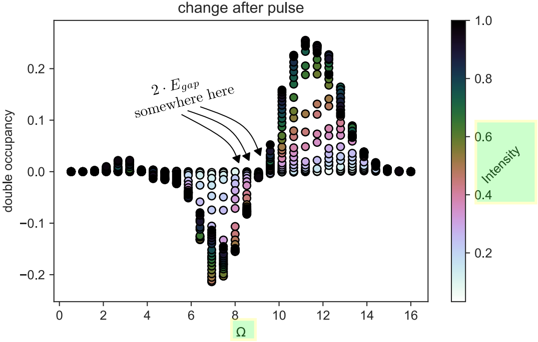
Results



0
E_{gap}
$2 \cdot E_{gap}$
$E_{gap} + 2 \cdot E_{bw}$
photon energy
$\Omega = 16.0$
double occupancy
0.55
0.50
0
50
100
150
200
250
300
t
double occupancy
0.550
0.525
0.500
0.475
0
10
20
30
PULSE
t
0.5190
0.5185
0.5180
0.5175
100
200
300
t

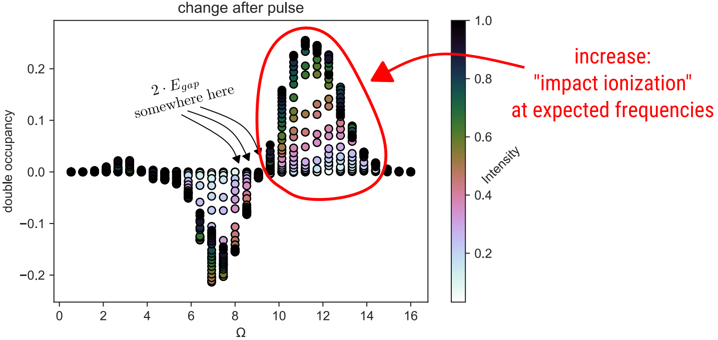
Change of Double Occupancy **AFTER** Pulse

Look at increase/decrease after pulse.



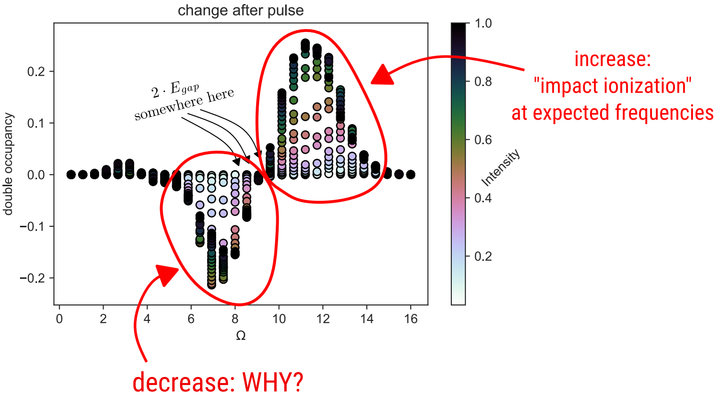
Change of Double Occupancy AFTER Pulse

Look at increase/decrease after pulse.



Change of Double Occupancy AFTER Pulse

Look at increase/decrease after pulse.



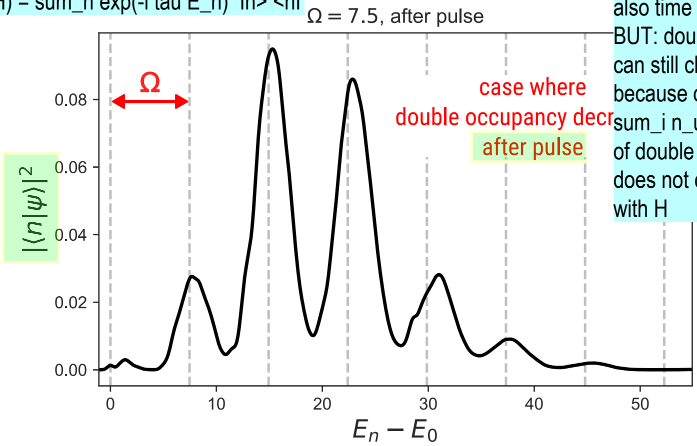
Spectrum in Eigenstates of $H(0)$: Multiphoton absorptions

Eigenstates |n> of H

$$\langle\psi(t)|\, e^{-i\tau H(0)} \underbrace{|\psi(t)\rangle}_{\text{after pulse}} \xrightarrow[\text{FT w.r.t. } \tau]{} \sum_{n\in\{ES\}} \delta\left(\omega - E_n\right)\ |\langle n|\psi(t)\rangle|^2$$

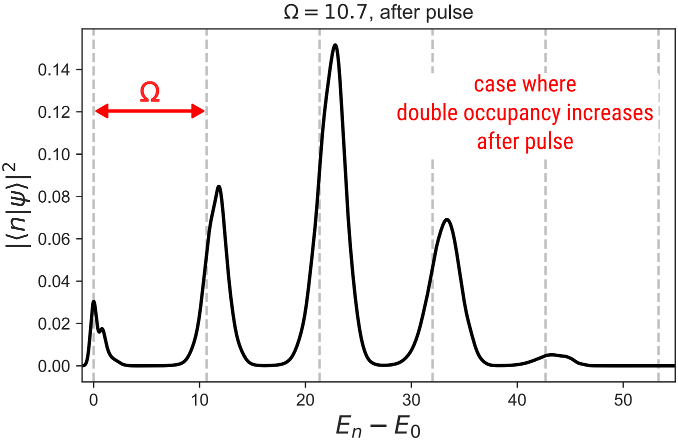
When H is time indep. then these coeff. are also time indep.
BUT: double occup. can still change, because oper. sum_i n_up,i n_down,i of double occupation does not commute with H

exp(-i tau H) = sum_n exp(-i tau E_n) |n> <n|



Spectrum in Eigenstates of $H(0)$: Multiphoton absorptions

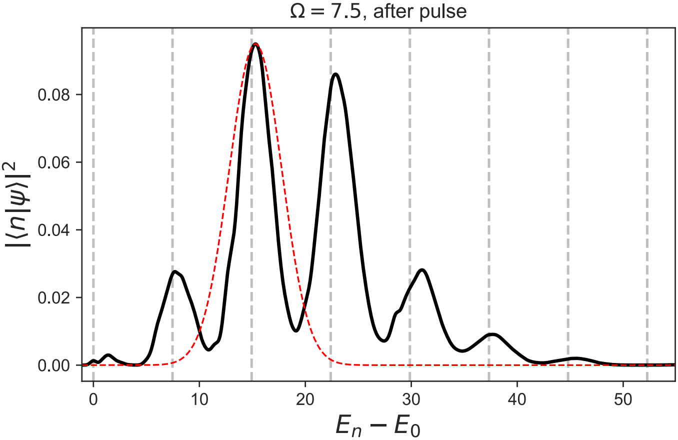
$$\langle\psi(t)|\, e^{-i\tau H(0)} \underbrace{|\psi(t)\rangle}_{\text{after pulse}} \xrightarrow[\text{FT w.r.t. } \tau]{} \sum_{n\in\{ES\}} \delta\left(\omega - E_n\right)\, |\langle n|\psi(t)\rangle|^2$$



Filtering: Extract Single Peak

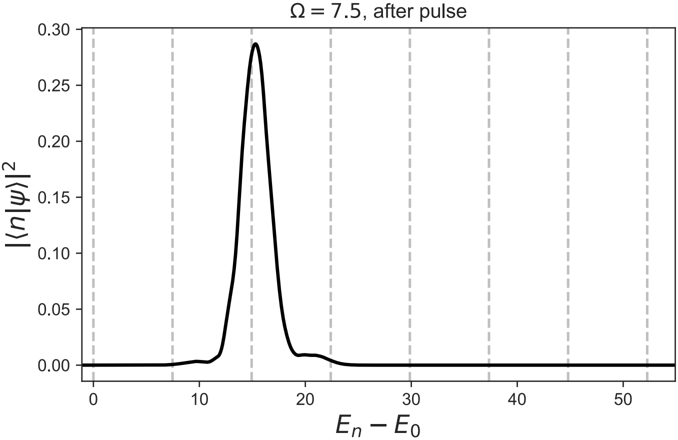
"time evolution" with auxil. time tau

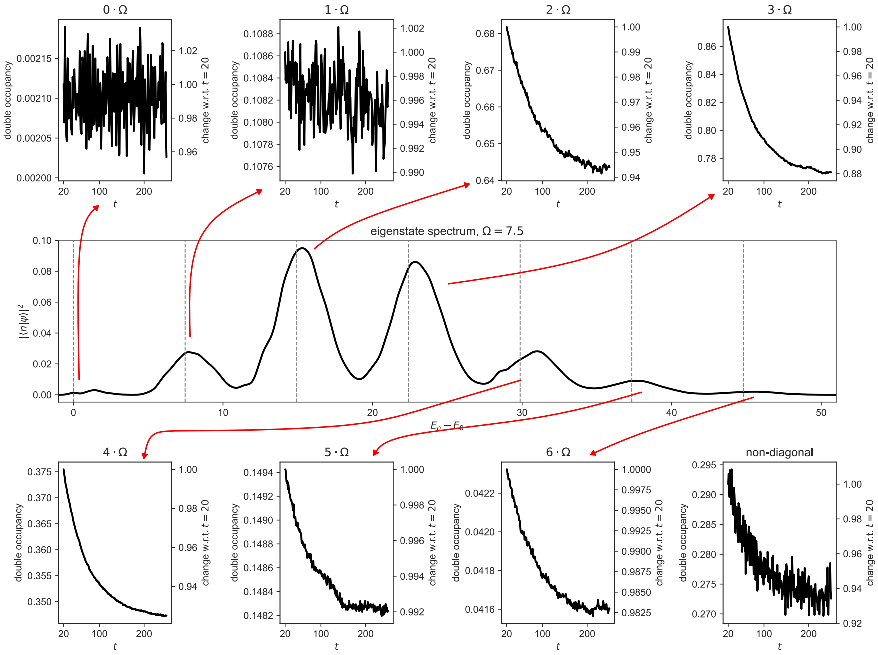
$$e^{-\tau(H-E_c)^2}\,|\psi(t)\rangle = \sum_{n\in\{ES\}} e^{-\tau(E_n-E_c)^2}\;\langle n\,|\,\psi(t)\rangle\;|n\rangle$$

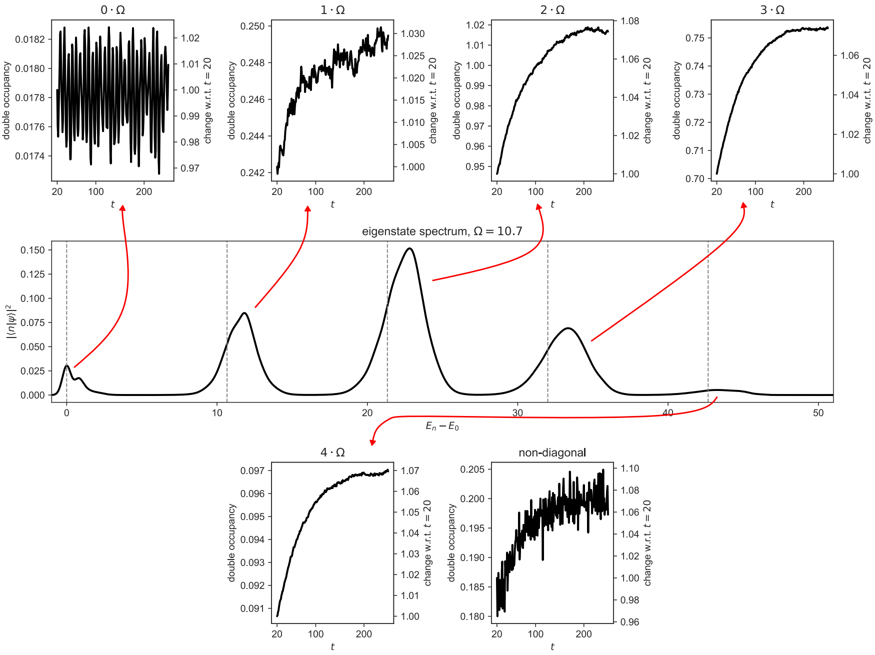


Filtering: Extract Single Peak

$$e^{-\tau (H-E_c)^2} |\psi(t)\rangle = \sum_{n \in \{ES\}} e^{-\tau (E_n - E_c)^2} \; \langle n \,|\, \psi(t) \rangle \; |n\rangle$$



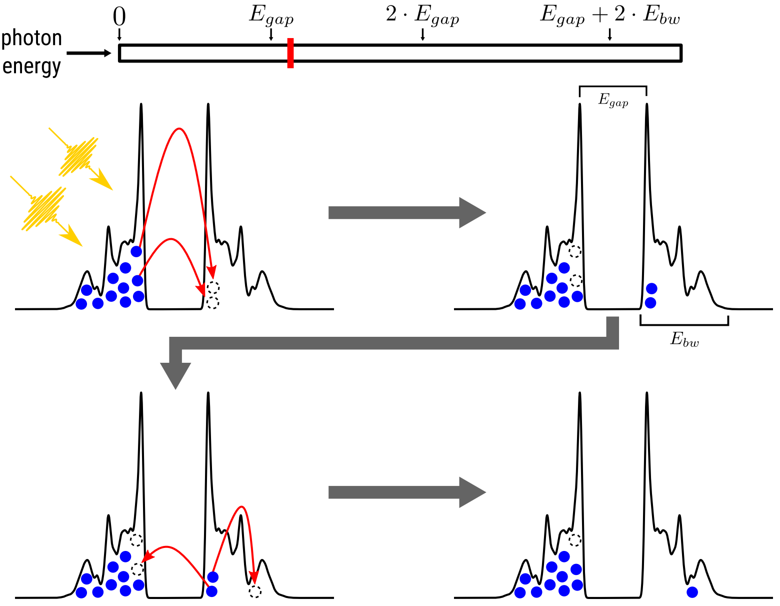

0 · Ω
1 · Ω
2 · Ω
3 · Ω
double occupancy
change w.r.t. t = 20
t
eigenstate spectrum, Ω = 7.5
|⟨n|ψ⟩|²
E_n − E_0
4 · Ω
5 · Ω
6 · Ω
non-diagonal



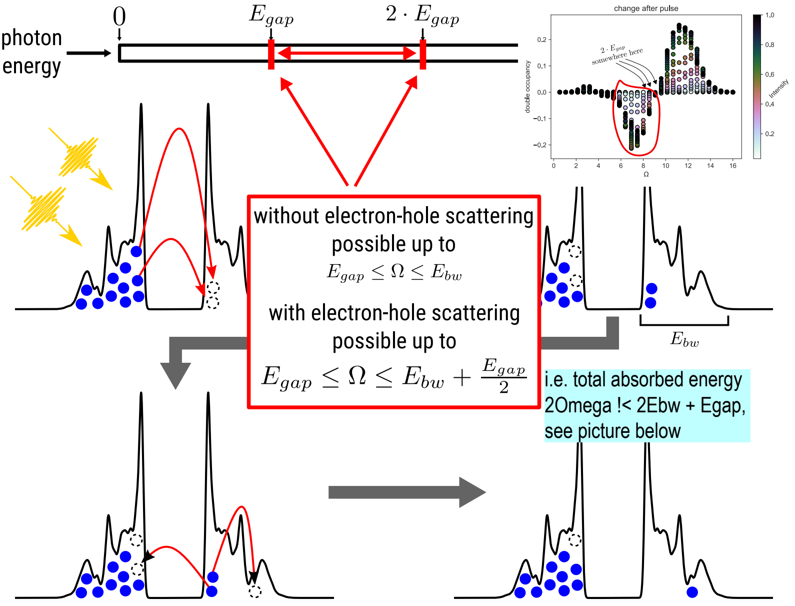
0 · Ω
1 · Ω
2 · Ω
3 · Ω
double occupancy
change w.r.t. t = 20
t
eigenstate spectrum, Ω = 10.7
|⟨n|ψ⟩|²
E_n − E_0
4 · Ω
non-diagonal

One Possible Explanation for "Deionization"

Auger recombination

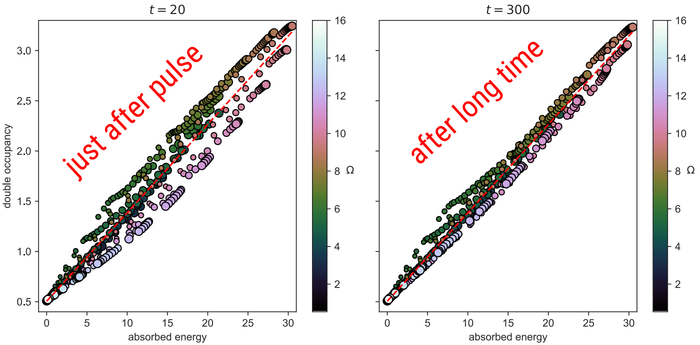


One Possible Explanation for "Deionization"



Results

Final double occupancy is depends almost only on absorbed energy.



Can be understood with process very similar to Eigenstate Thermalization Hypothesis.

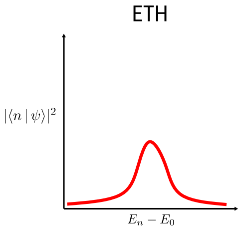
Eigenstate Thermalization Hypothesis

$$\overline{\langle O(t) \rangle} = \frac{1}{t} \int_0^t \langle O(\tau) \rangle \, \mathrm{d}\tau$$

$$\xrightarrow[t \gg 0]{} \sum_n \langle n \,|\, O \,|\, n \rangle \; |\langle n \,|\, \psi \rangle|^2 \;\stackrel{?}{=}\; \sum_{\substack{n \\ |E_n - E_\psi| < \Delta E}} \langle n \,|\, O \,|\, n \rangle$$

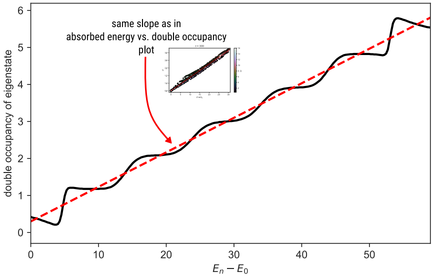
Possible Explanation: For two eigenstates $|n\rangle$ and $|m\rangle$:

$$E_n \approx E_m \Longrightarrow \langle n \,|\, O \,|\, n \rangle \approx \langle m \,|\, O \,|\, m \rangle$$



Expectation value of Eigenstates

Expectation value of double occupancy can be estimated with random sampling and filtering.

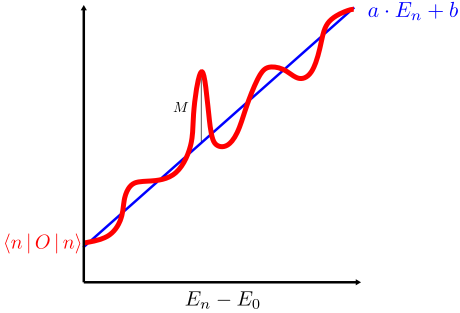


We find that the resulting slope is the same as before. Composite states have the same expectation value as eigenstates?

"Linear ETH"

Assumption:

$$\langle n \,|\, O \,|\, n \rangle = a \cdot E_n + b + \epsilon(E_n)$$
$$|\epsilon(E_n)| \leq M$$



Then:

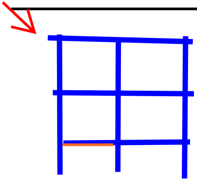
$$\left| \overline{\langle O \rangle} - a \cdot \langle H \rangle - b \right| \leq M$$

Summary

- 4×3 Hubbard model, excited with "light pulse" (Peierls phase).
- We see growing and shrinking of double occupancy after pulse.
- On a quasi-particle level a possible explanation is "impact ionization" and "deionization".
- On the eigenstate level we see an ETH-like process.

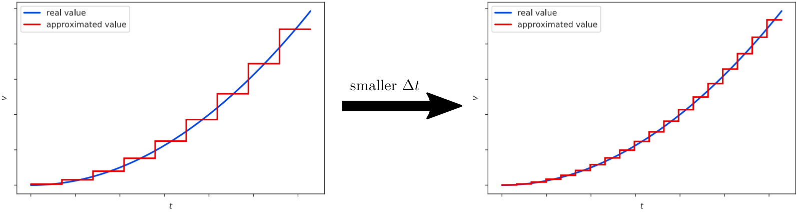
Thank you very much for your attention!

Numerical Details



exp(-i H(t) delta-t) approx 1 - i H(t) delta-t

$$\mathcal{T} e^{-i \int_{t_0}^{t_0+\Delta t} H(t)\, dt} \approx e^{-i \frac{1}{2}(H(t_0)+H(t_0+\Delta t))\, \Delta t}$$



We checked for convergence with different Δt.